

# Molecular Dynamics Simulations of Supercritical Jet Mixing

M. M. Micci, Maj. R. D. Branam and K. F. Ludwig

Department of Aerospace Engineering

The Pennsylvania State University

University Park, PA 16802

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# Introduction

- High pressure heterogeneous combustion systems typically operate trans- or supercritical
  - Liquid rocket engines
  - Gas turbine combustors
  - Diesel engines
- Quantitative assessments or validated theories characterizing propellant injection at near and supercritical conditions are currently limited



Vulcain



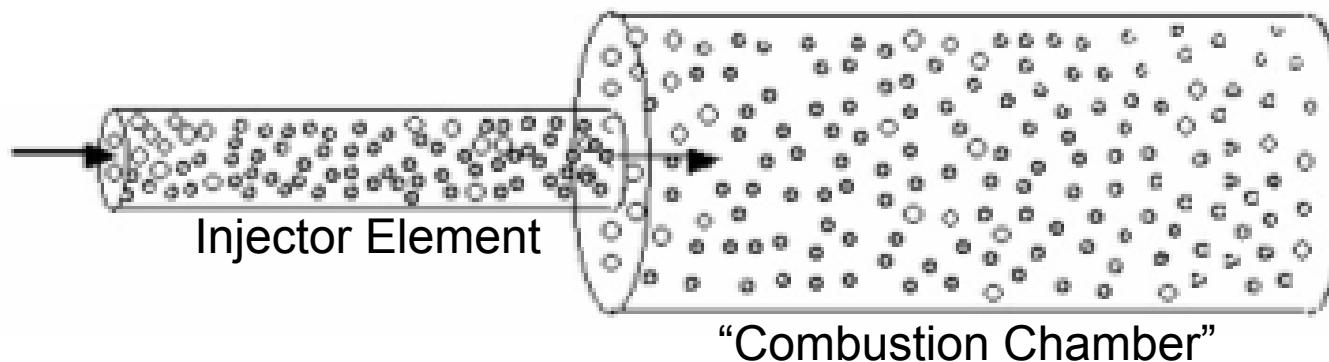
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# Introduction

- Because these systems operate at near and supercritical conditions, it is difficult to model the injection, mixing, atomization, and vaporization using traditional CFD
  - System becomes fully 3-D
  - Material and transport properties change significantly
  - Moves from 2-phase to 1-phase
  - Complex mixture effects

# Introduction

- This research attempts to address these limitations through the use of MD as an alternate simulation tool
- Diatomic liquid nitrogen ( $N_2$ ) is simulated as a non-reacting substitute to other diatomic cryogenic liquid propellants/oxidizers, i.e.  $H_2$  or  $O_2$   
Experimental database exists
- The simulation consists of two cylinders
  - Smaller diameter cylinder representing one injector through which simulated liquid nitrogen flows
  - Larger diameter cylinder of gaseous nitrogen into which the simulated



# Introduction

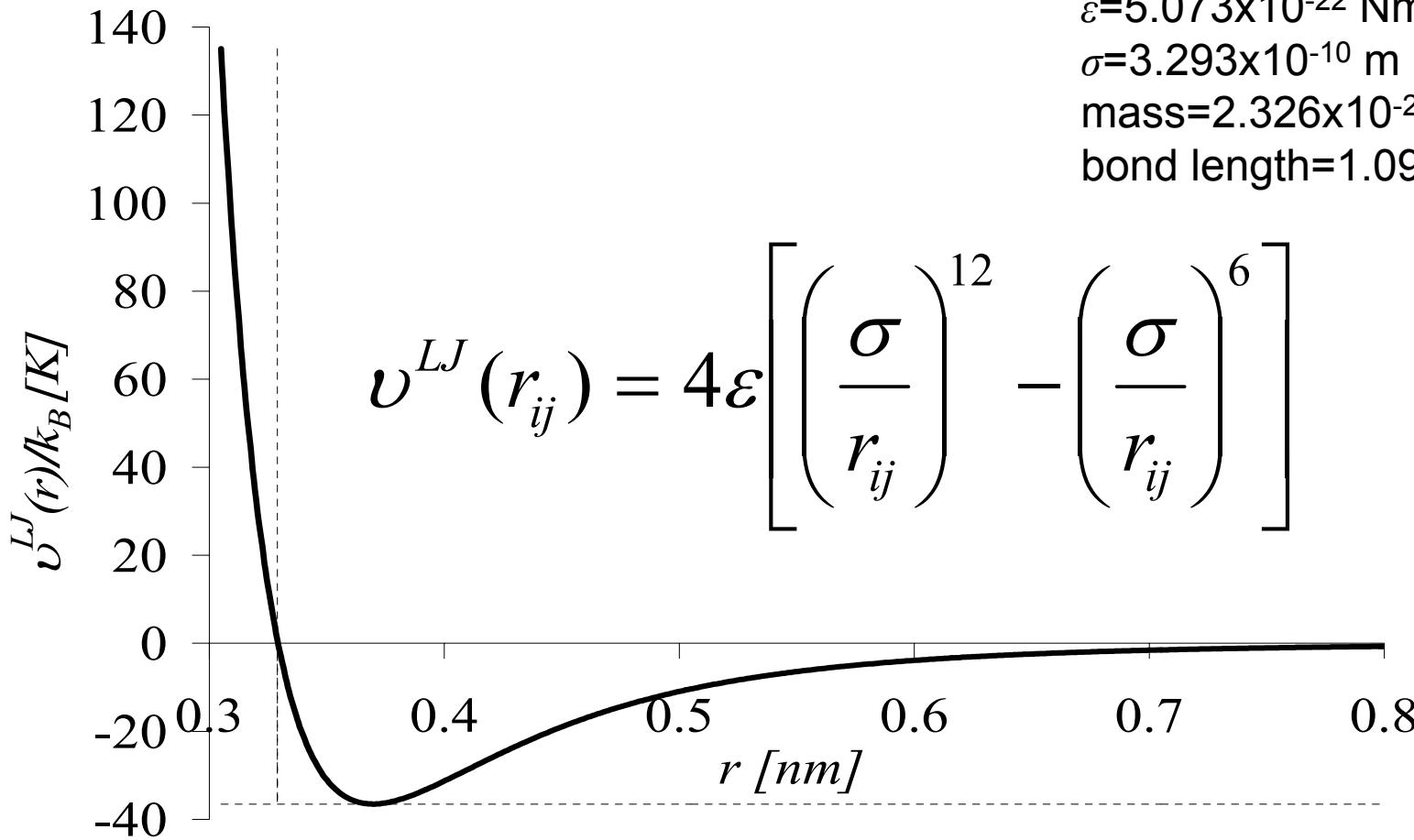
- Advantages of the MD model:
  - Based purely on first principles ( $F=ma$ )
  - Can theoretically span all conditions; no need to track phase boundaries
  - Geometric assumptions do not need to be made
  - Equation of state, material and transport properties are not needed, and *can actually be* calculated outputs
  - Mixture effects automatically incorporated

# Fundamental Concepts of MD

- Dynamics of interest is contained within solution to the classical N-body problem
- MD is a numerical tool used to solve Newton's Laws of Motion, applied to motions of individual atoms or molecules
  - $F = ma$  is the only equation to solve
  - Forces on atoms derived from interatomic potentials

# Fundamental Concepts of MD

## ■ Lennard-Jones 12-6 Potential



For Nitrogen Atoms:

$$\epsilon = 5.073 \times 10^{-22} \text{ Nm}$$

$$\sigma = 3.293 \times 10^{-10} \text{ m}$$

$$\text{mass} = 2.326 \times 10^{-26} \text{ kg}$$

$$\text{bond length} = 1.094 \times 10^{-10} \text{ m}$$

# Fundamental Concepts of MD

- Equations of Motion

$$m_a \mathbf{a}_i = \mathbf{F}_i = \sum_{j=1}^{N_a} \mathbf{f}_{ij}$$

- For Lennard-Jones Potential

$$\mathbf{f} = -\nabla v^{LJ}(r)$$

$$\mathbf{f}_{ij} = \left( \frac{48\varepsilon}{\sigma^2} \right) \left[ \left( \frac{\sigma}{r_{ij}} \right)^{14} - \frac{1}{2} \left( \frac{\sigma}{r_{ij}} \right)^8 \right] \mathbf{r}$$

- Solve Numerically Using Finite Difference Velocity-Verlet Algorithm

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \Delta t \mathbf{v}(t) + \frac{\Delta t^2 \mathbf{a}(t)}{2}$$

$$\mathbf{v}(t + \Delta t / 2) = \mathbf{v}(t) + \frac{\Delta t \mathbf{a}(t)}{2}$$

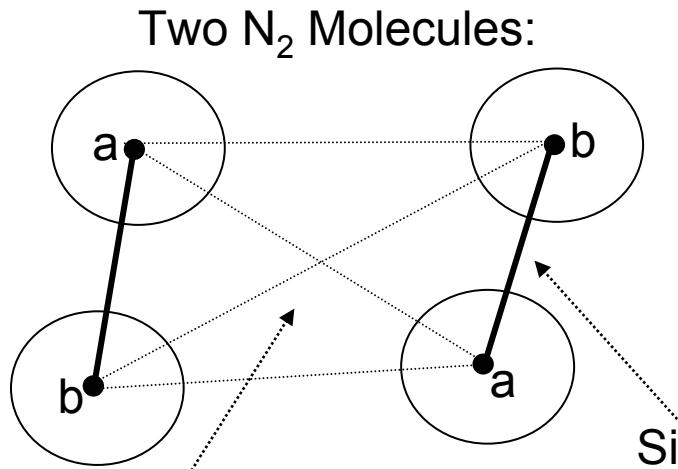
$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \Delta t / 2) + \frac{\Delta t \mathbf{a}(t + \Delta t)}{2}$$

# Fundamental Concepts of MD

- Addition of Bond Constraint to Simulate Diatomic Nitrogen Molecule

$$r_{ab}^2 = \mathbf{r}_{ab} \cdot \mathbf{r}_{ab} = \text{constant}$$

$$\frac{d(r_{ab}^2)}{dt} = 2\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} = 0$$



RATTLE Algorithm:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}'(t + \Delta t) + \left( \frac{\Delta t^2}{2m} \right) \mathbf{g}(t)$$

$$\mathbf{v}(t + \Delta t / 2) = \mathbf{v}'(t + \Delta t / 2) + \left( \frac{\Delta t}{2m} \right) \mathbf{g}(t)$$

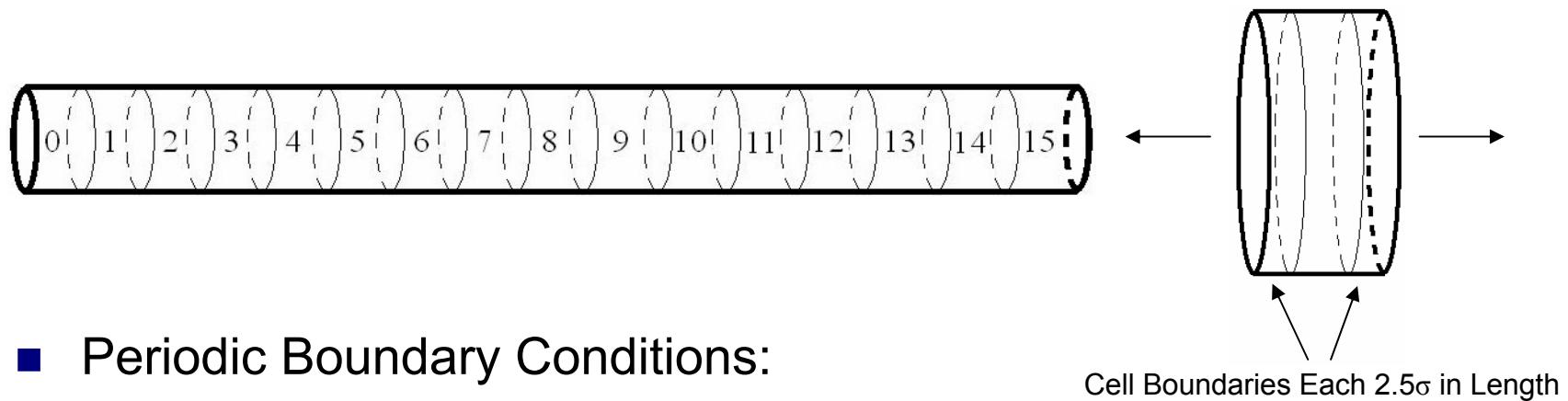
$$\mathbf{v}(t + \Delta t) = \mathbf{v}'(t + \Delta t) + \left( \frac{\Delta t}{2m} \right) \mathbf{g}(t + \Delta t)$$

Simulated bond using RATTLE

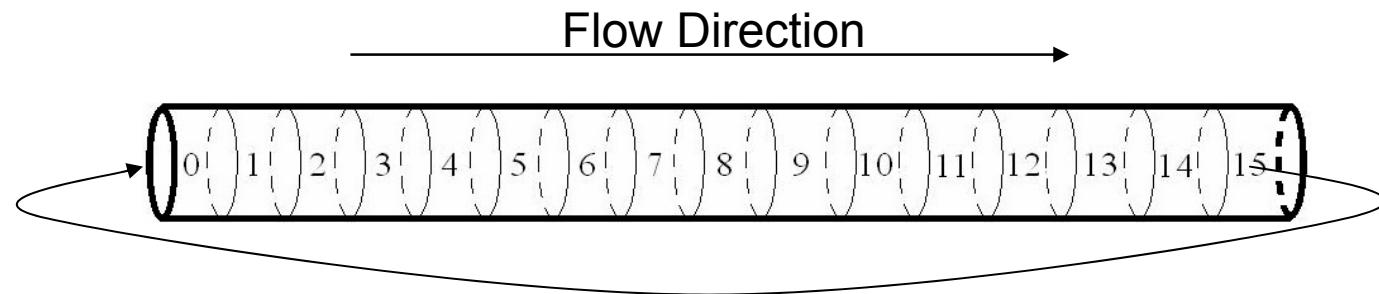
# Simulation Methodology

## ■ Computational Domain and Processor Setup:

- Each processor assigned to handle particles within a specific geometric region
- As particles move, they are transferred between processors

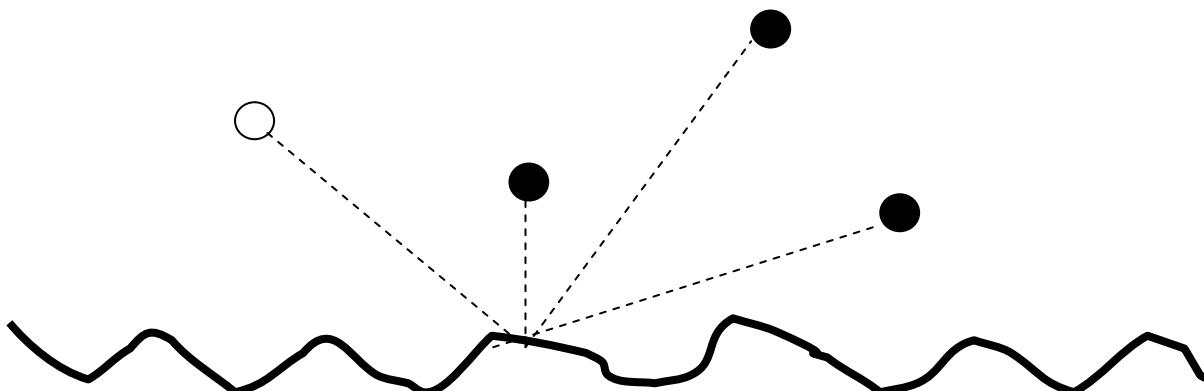


## ■ Periodic Boundary Conditions:

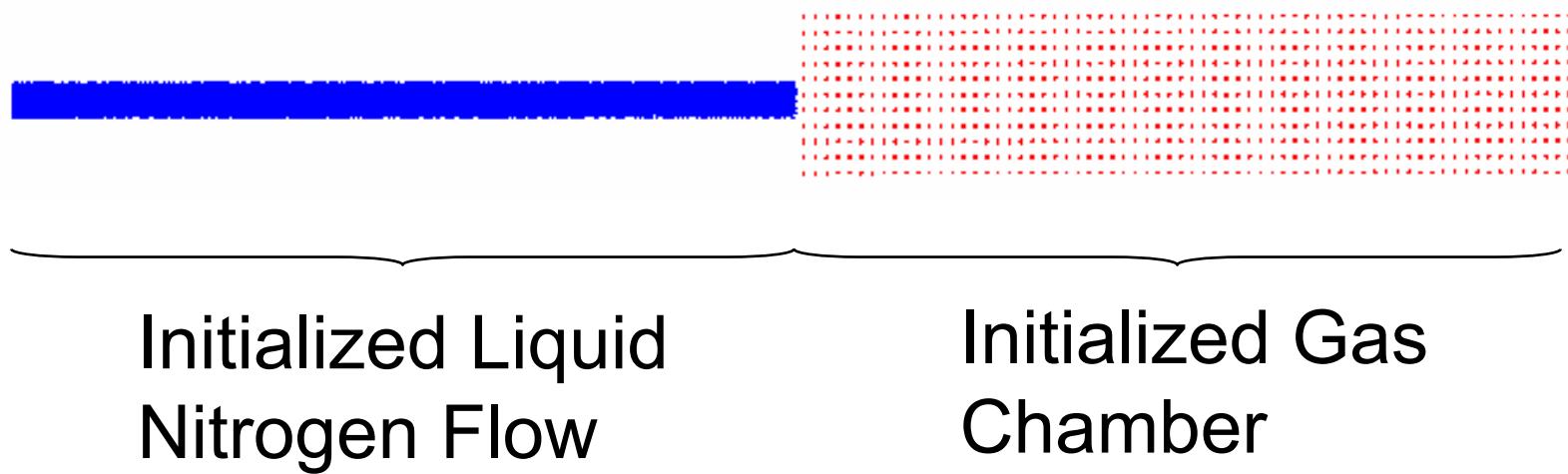


# Wall Model

- Constant Temperature Wall
- Diffusely Reflecting
  - Molecules reemitted from wall in random direction with random velocity based on Maxwellian distribution scaled to the wall temperature.
  - Removes heat generated by viscous dissipation



# Simulation Methodology



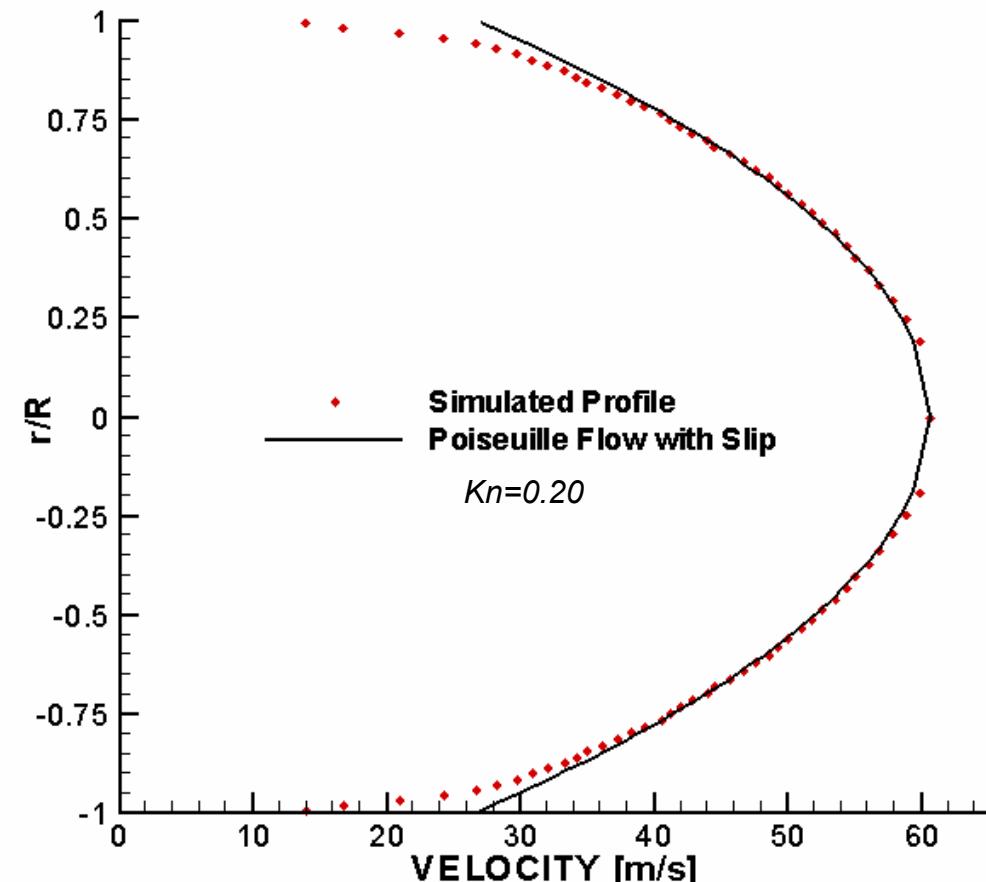
# Results

## Velocity Profile

$$\lambda = \frac{1}{\sqrt{2\pi} d^2 n} \quad Kn = \frac{\lambda}{L}$$

$$u(r) = u_{\max} - \frac{u_{\max}}{1 + 4Kn} \left( \frac{r}{R} \right)^2$$

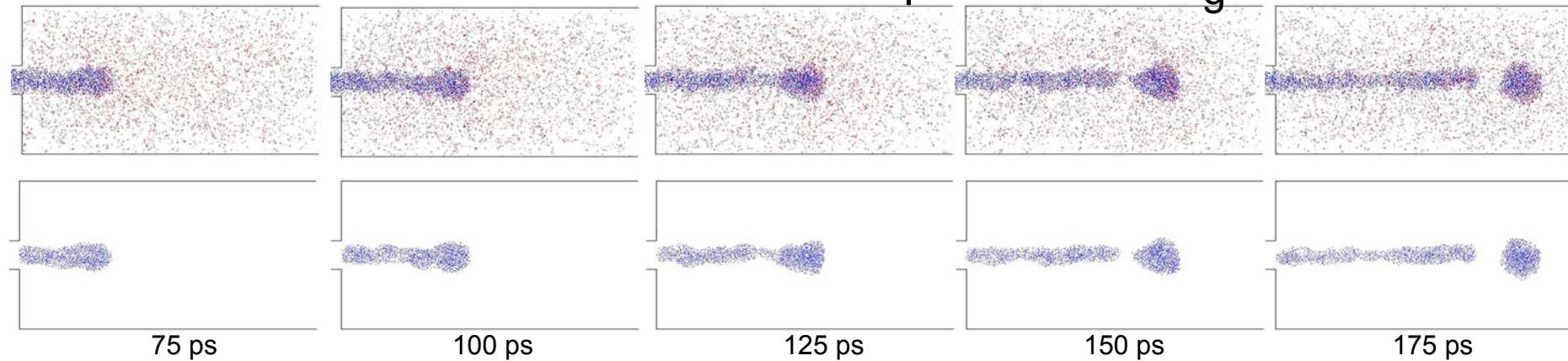
$$u(R) = -\lambda \left( \frac{du}{dr} \right)_{r=R}$$



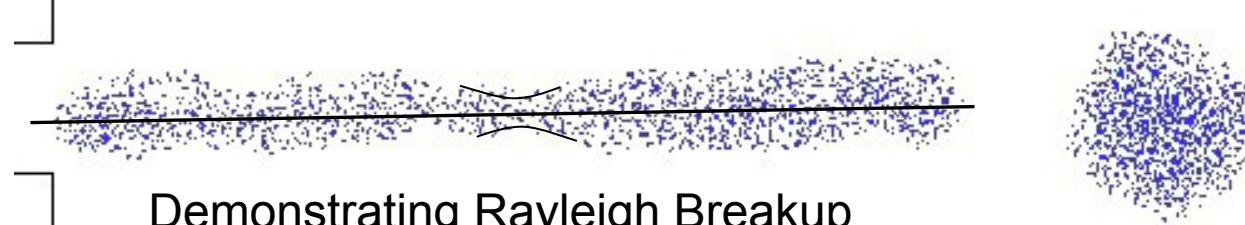
Radial Velocity Profile

# Results

■ 94 K, ~0.5 MPa, Re=1.63, We<sub>l</sub>=1.50, We<sub>g</sub>=0.04



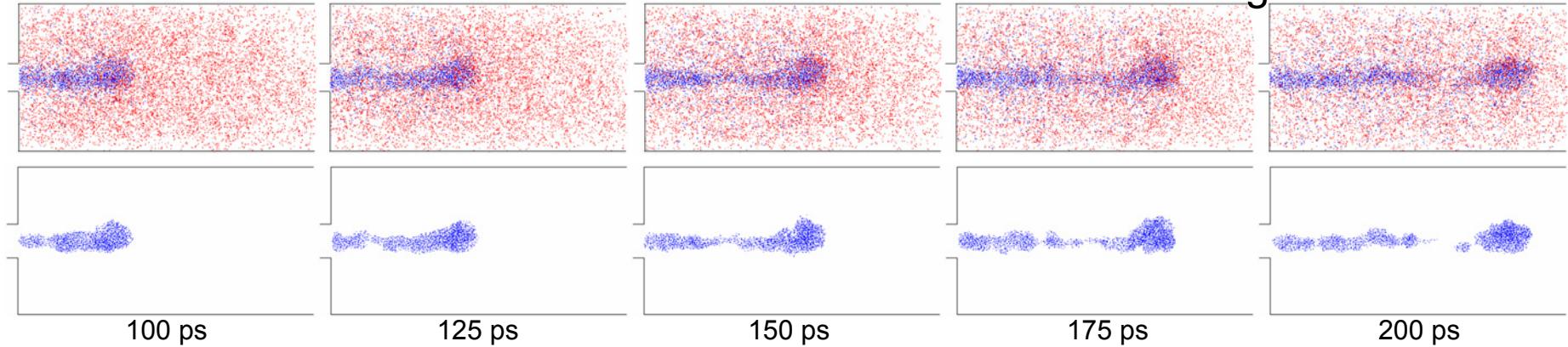
Source: Mayer, W. O., and Telaar, J., "Investigation of Breakup of Turbulent Cryogenic Variable-Density Jets." *Atomization and Sprays*, **12**, 651-666, 2002.



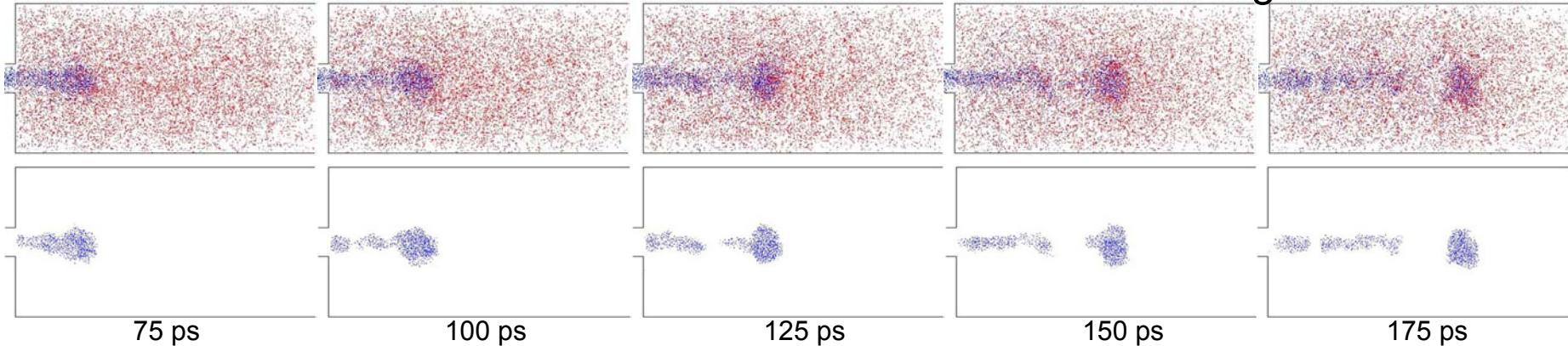
Demonstrating Rayleigh Breakup

# Results

- 104 K, ~1.0 MPa, Re=2.07, We<sub>l</sub>=2.18, We<sub>g</sub>=0.14

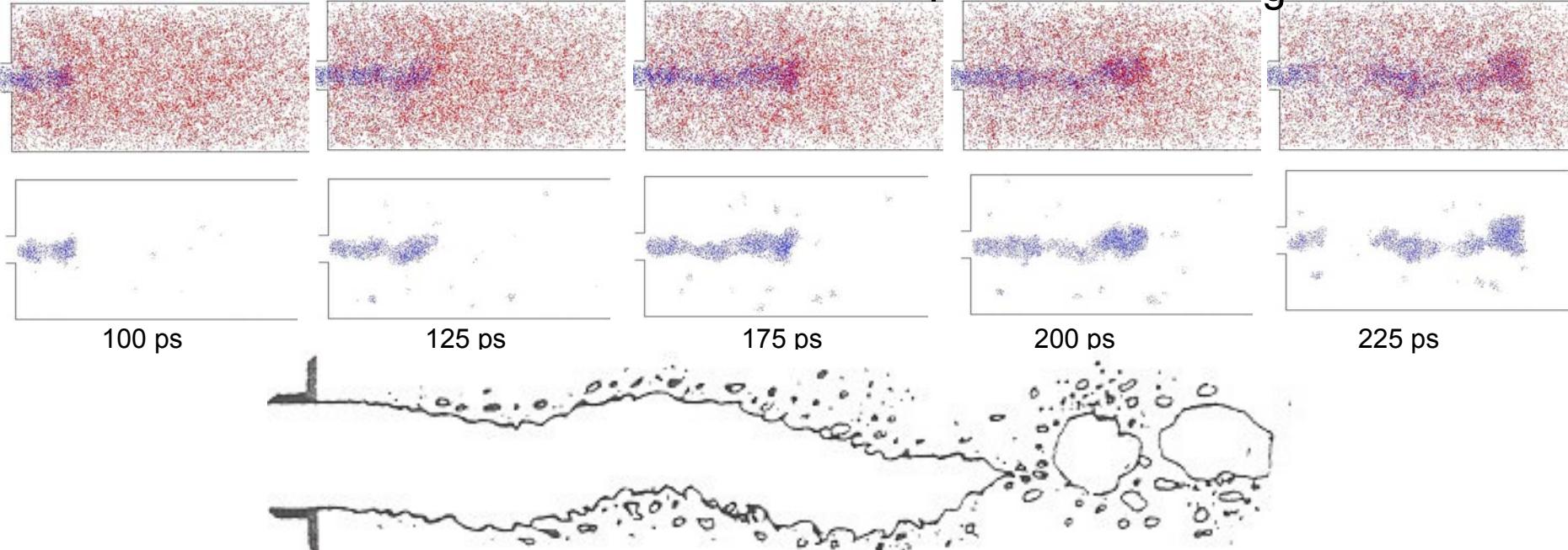


- 114 K, ~2.0 MPa, Re=2.71, We<sub>l</sub>=4.62, We<sub>g</sub>=0.45

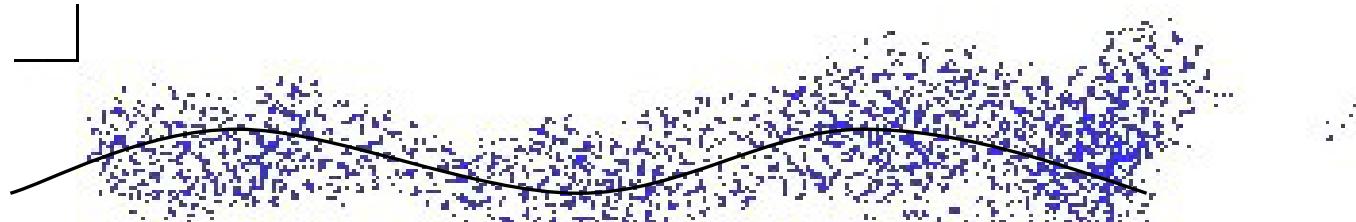


# Results

- 124 K, ~3.0 MPa, Re=4.04, We<sub>l</sub>=41.53, We<sub>g</sub>=7.06

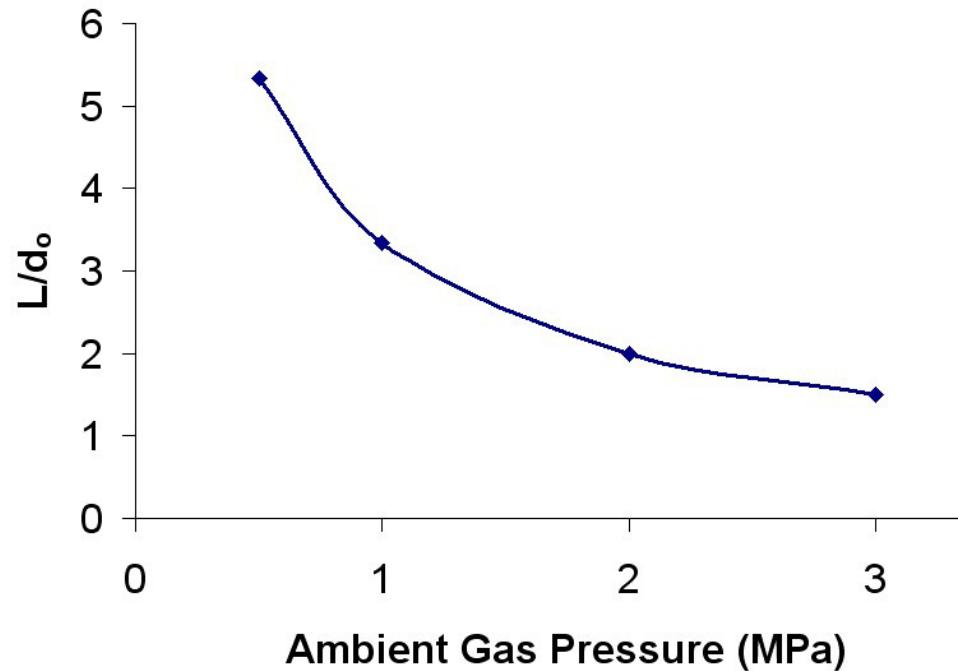


Source: Mayer, W. O., and Telaar, J., "Investigation of Breakup of Turbulent Cryogenic Variable-Density Jets." *Atomization and Sprays*, 12, 651-666, 2002



Demonstrating Second Wind-Induced Breakup

# Results



- A decrease in breakup length with an increase in ambient pressure is observed
- The difference in breakup length between the higher ambient pressure cases is also less, indicative of higher pressures having less of an effect on breakup length

# Animation

83 K

~0.2 MPa

$Re=1.09$

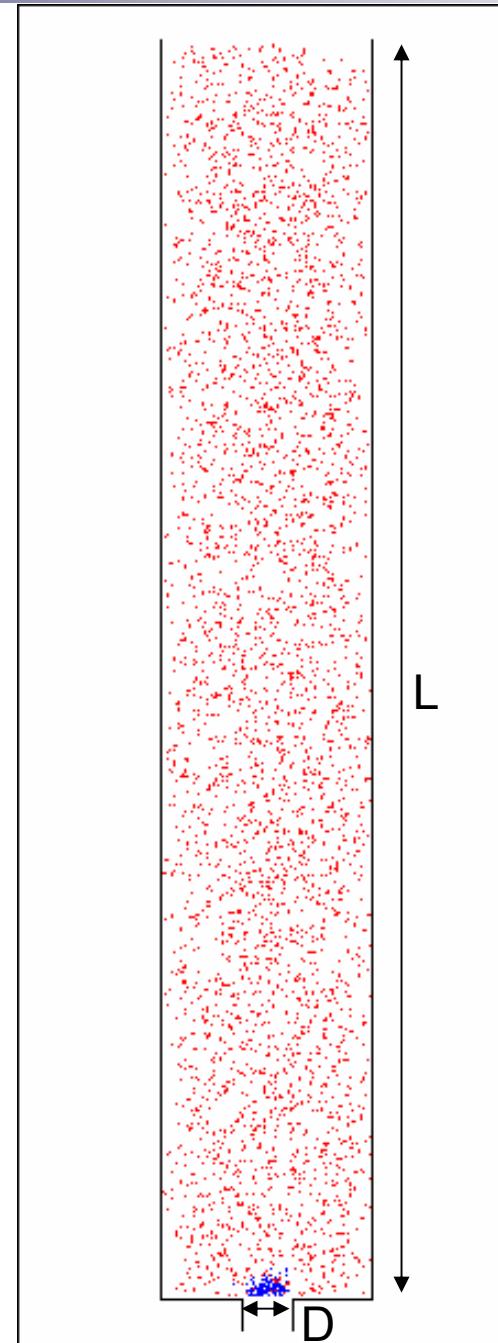
$We_l=0.84$

$We_g=0.009$

$u_{avg}=45.3 \text{ m/s}$

$L/D=60$

Total Simulation Time:  
1.2625 ns



Case1prev\_nf.avi

# Animation

83 K

~0.2 MPa

$Re = (a) 0.87, (b) 1.70$

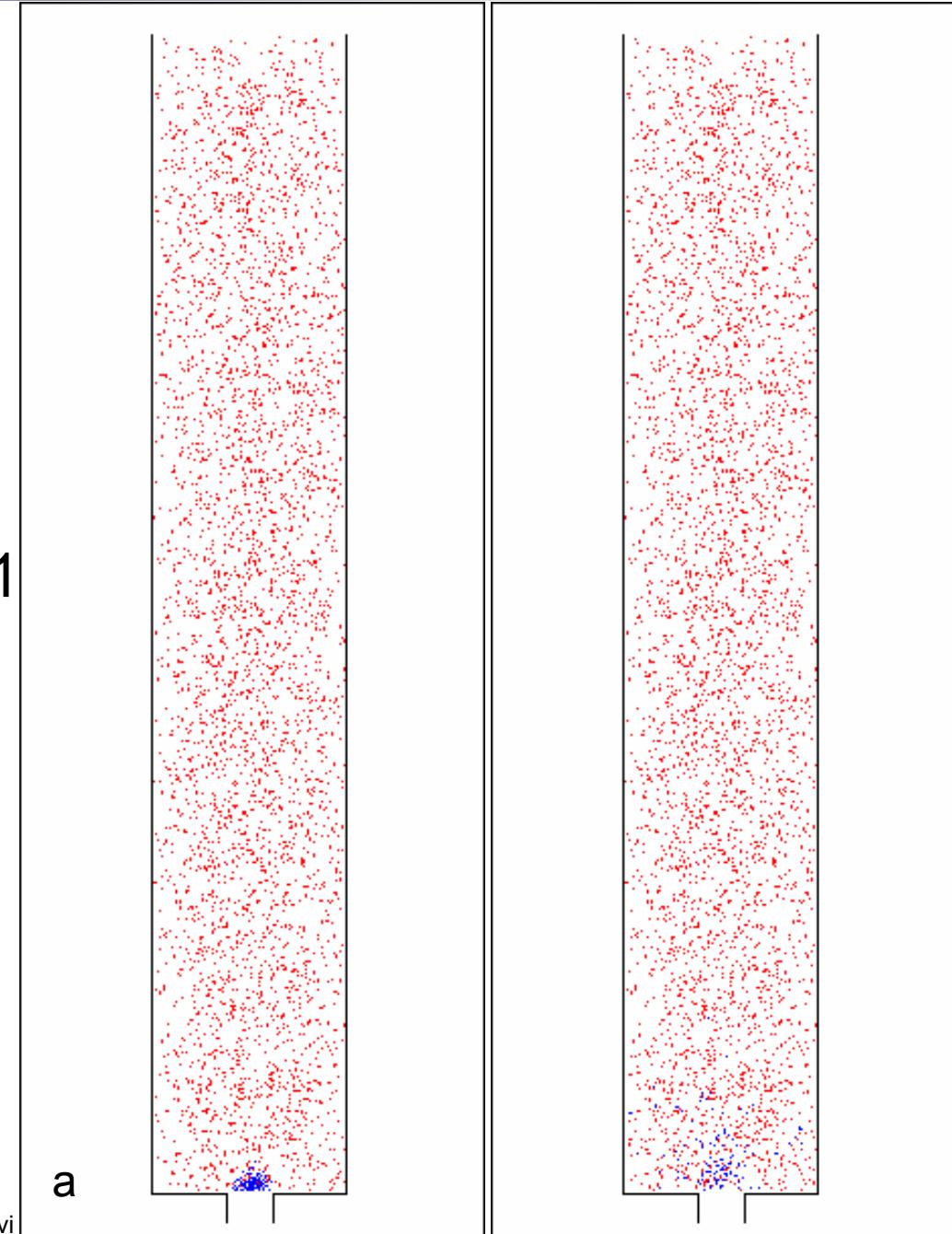
$We_l = (a) 0.50, (b) 1.90$

$We_g = (a) 0.005, (b) 0.021$

$u_{avg} = (a) 33.8 \text{ m/s}$   
 $(b) 66.1 \text{ m/s}$

$L/D = 60$

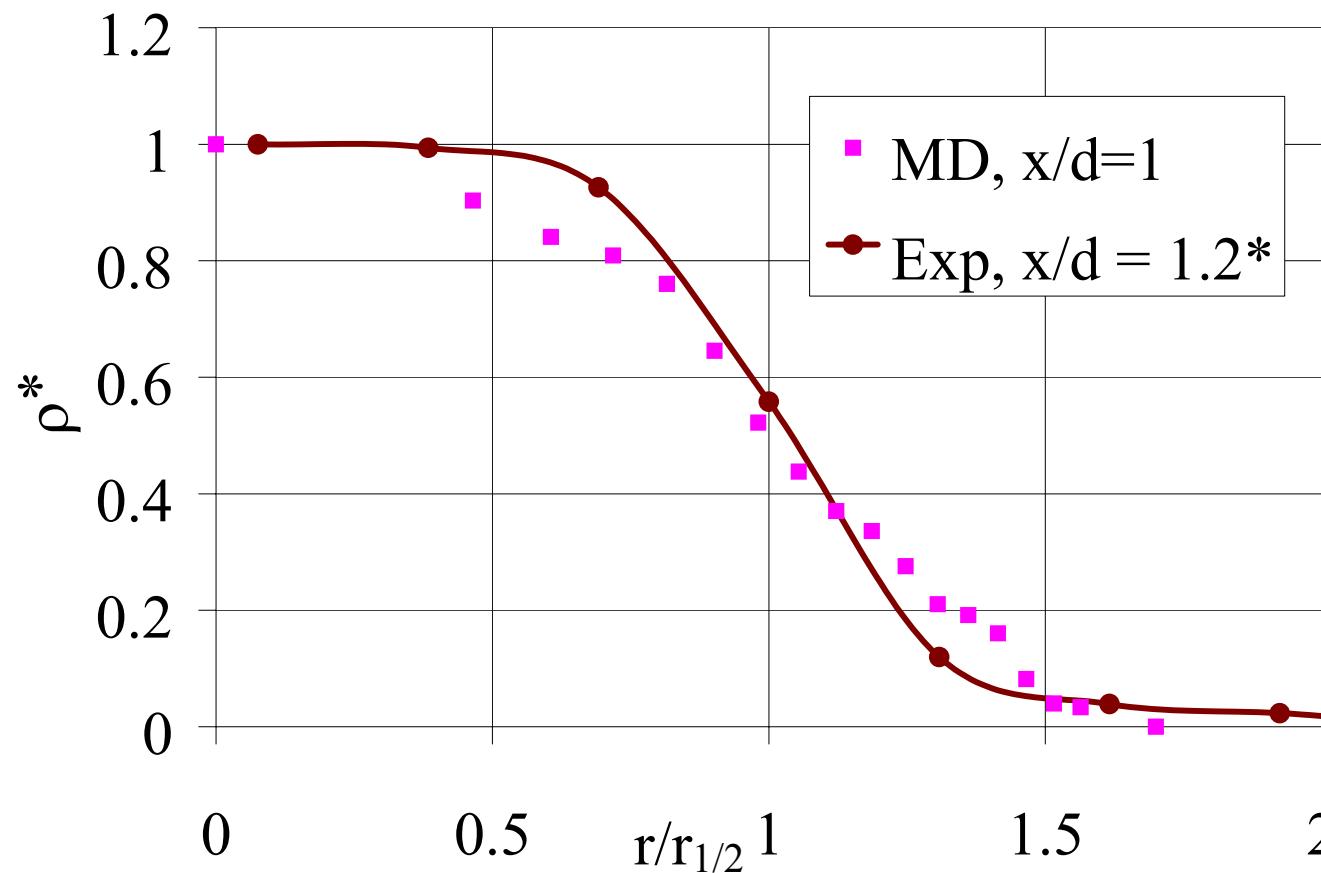
Total Simulation Time:  
1.2625 ns



(a) Case1new.avi, (b) fgrav2xspray.avi

# Supercritical - Comparison to Raman measurement

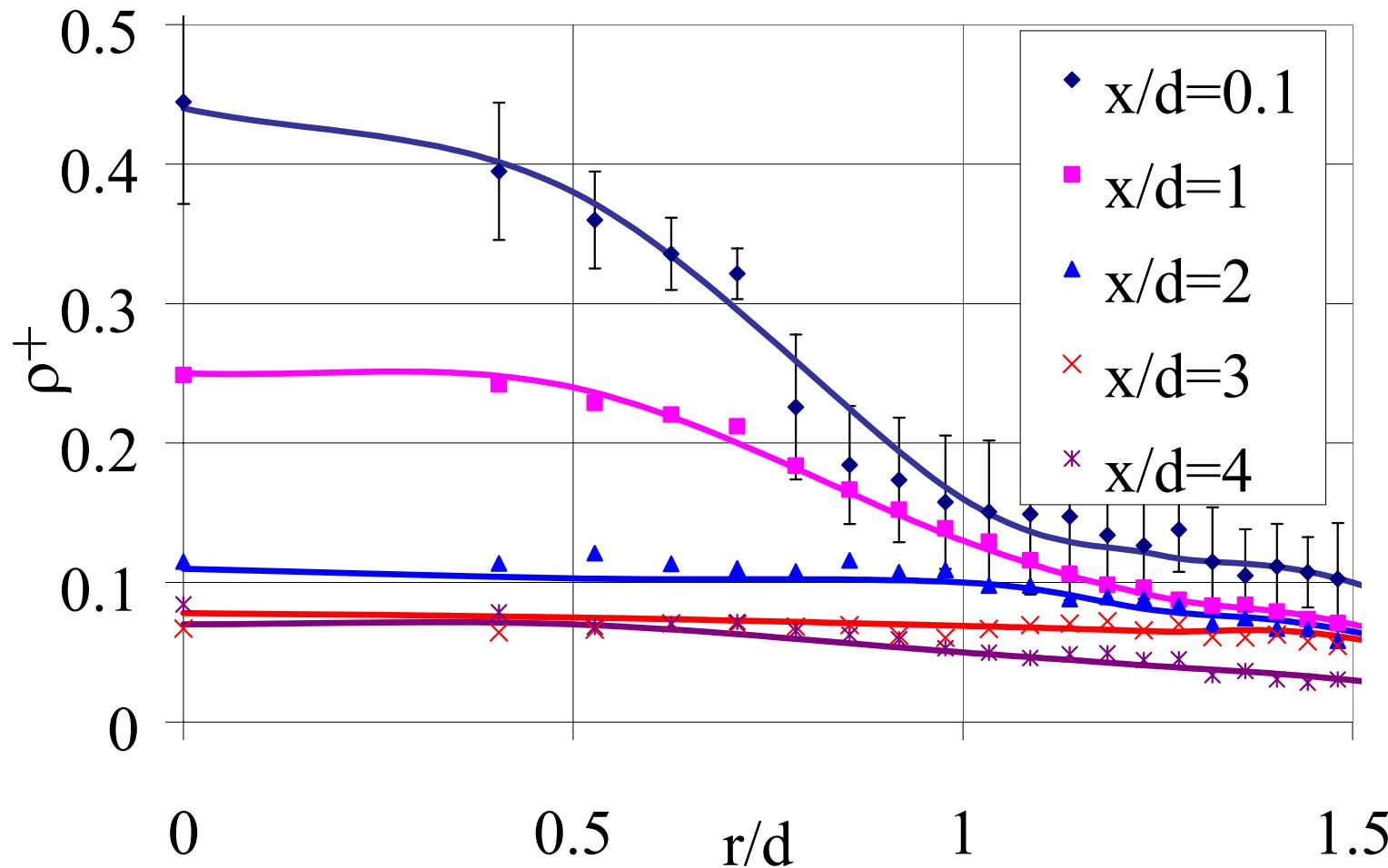
■ 4 MPa, 123 K



\*Branam, R. and Mayer, W., "Characterization of Cryogenic Injection at Supercritical Pressure," *J. Prop. and Pow.*, Vol. 19, No. 3, May-June 2003, pp. 342-355.

# Supercritical - Computed radial density profiles

- Target conditions, 6 MPa, 123 K, 40 m/s

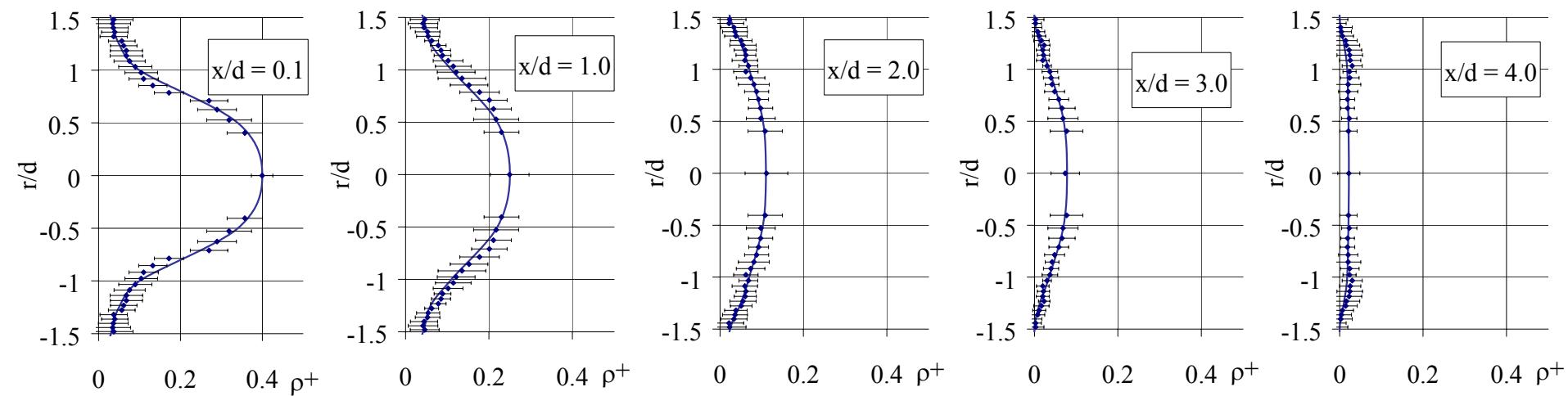


# Supercritical - Evolution of computed density profiles

## ■ Developing Flow

- At a given time
- Average of five independent simulations

## ■ Supercritical conditions, 4 MPa, 123 K



# Summary

## ■ Subcritical Injection Simulations:

- Rayleigh breakup is reproduced, resulting in formation of droplets due to capillary instabilities in the jet driven by surface tension
- The onset of aerodynamic effects, including the second wind-induced breakup regime, can also be seen in the cases of higher gas pressures

# Summary (II)

- Supercritical Injection Simulations:
  - MD simulations match Raman measurements near injector exit (potential core)
  - Simulated flow still transient further downstream

# Future work

- Resolve wall B.C. rotational accommodation
- Increase size of simulations
  - Generating injected particles
  - Increase tube diameter
  - Increase Re, decrease Kn
- Future work to focus more on ethanol and other hydrocarbons
- Extend geometry to include coaxial tube



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